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A Dynamic Model for Glucose Fermentation in a Three-Phase Bioreactor

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Abstract

In this study the performance of an special three-phase bioreactor for biological production of ethanol and hydrogen was modeled using computational fluid dynamics. The effect of different Hydraulic Retention Time (HRT) of 1, 2 and 4 hr and Glucose mass fraction in feed of 0.002, 0.004, 0.006, and 0.008 on Hydrogen and ethanol production rate was determined. The maximum value of H_2 production rate at the HRT of equal to 2h and Glucose mass fraction of 0.008 is 0.033 kg/h. It was demonstrated that the model is capable of predicting the variation of the EGSB reactor performance for biohydrogen and bioethanol production at various substrate concentrations and HRT values.

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1. Introduction

One of the most important challenges of the current century is to develop new sources of renewable energies which might be able to replace fossil fuels. An ideal replacement would be a clean fuel that has a high efficiency of conversion. Hydrogen is a promising fuel because it is clean, renewable, and has a high energy density of 122 kJ/gr [1]. Currently, hydrogen is produced by electrolysis of water or by steam reformation of methane amongst other techniques. Unfortunately, most of these processes are highly energy intensive, making hydrogen production very expensive [2, 3]. Biological H_2 production as an alternative route

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is more attractive especially when organic wastewater or other wastes are used as raw materials. Under anaerobic conditions, hydrogen is produced as a by-product during the conversion of organic wastes into organic acids, which are then used for methane generation. The acidogenic phase of anaerobic digestion can be manipulated to improve H_2 production [2,3]. The anaerobic digestion is a multi-step process consisting of hydrolysis of complex organic substrates such as proteins, lipids, and carbohydrates into soluble amino acids, fatty acids, and sugars followed by the fermentation to acetate, format, hydrogen, and carbon dioxide, which are finally utilized by methanogenic microorganisms to form methane. Anaerobic reactors such as upflow anaerobic sludge blanket (UASB), expanded granular sludge bed (EGSB) and anaerobic fluidized bed (AFB) reactors are commonly used for the biological processes.[4,5,6,7].

The EGSB reactor, a three-phase system, has been widely used for the treatment of wastewater due to its high operational efficiency even at high organic loading rates (OLR) and heavy biomass accumulation on the support media [4]. Although an EGSB bioreactor has been used in biochemical applications for many years, but a restricted research have been published on its mathematical modeling. Because of the higher upflow velocities, which are caused by a high recycle rate and the sludge expansion through the whole reactor, which is caused by high height/diameter ratio, an EGSB reactor has minimum reactor dead volume.

2. Mathematical Modeling

2.1. Biochemical reaction

In this work, it is assumed that the fermentation process will immediately take place as the water is contacted with the sludge phase in a reactor with height of 120 cm and the internal diameter of 6 cm [8]. The species reaction model was implemented to determine the mass fractions of glucose, ethanol, acetic acid, carbon dioxide, and hydrogen resulting from glucose fermentation, i.e.;



The rate equation for the reaction is written as:

$$R = -kC_{C_6H_{12}O_6} \quad (2)$$

With the reaction rate constant of 2.06 h^{-1} [7].

2.2. Turbulence modeling of the Continuous phase

The turbulence modeling of the continuous phase is based on the two-equation (k,ϵ) turbulence model derived in a three-phase flow, including the interfacial transfer of turbulent kinetic energy and its dissipation rate. The interphase momentum transfer between the two dispersed phases, as well as virtual mass force and turbulent dispersion force between the continuous phase and the dispersed phases are all neglected in this study.

2.3. Numerical solution

The finite volume method is used as the numerical technique. The momentum and continuity equations are discretized using finite volumes. For efficient use of computational time, our simulation of the EGSB reactor exploits the symmetric geometry of the reactor and simulates half the geometry in a two-dimensional surface. The simulation results vary little with grid density so truncation errors in the numerical simulation can be neglected. The geometry and the meshes are generated by an in-house code. Therefore, a two-dimensional

computational domain of the complete geometry of the EGSB reactor was devised with 14,440 cells, 29,780 faces, and 15,341 nodes and the solution of the model is independent from the number of them. The initial sludge bed was packed with granular solids with a volume fraction of 0.5.

The reactor wastewater inlet was modeled with a velocity-inlet boundary condition, and the outlet was set as a pressure outlet boundary condition. All other solid surfaces were defined by wall boundary conditions with no slip.

The simulation was operated in unsteady state conditions with time step sides equal to 0.001 s. The convergent solution was defined as the solution for which the normalized residual for all variables was less than 1×10^{-3} , except continuity that was less than 1×10^{-4} and the calculated outflow rate had reached a constant value.

To obtain hydrodynamic information from the EGSB reactor, six unsteady state simulations at different up-flow velocity matched to hydraulic retention time (HRT) and mass fraction of glucose were conducted in Table 1.

Table 1. Operating Conditions applied in this research

Working condition	Inlet velocity (m/s)	HRT (h)	Mass fraction of Glucose in feed
C1	0.014	1	0.008
C2	0.0069	2	0.008
C3	0.0034	4	0.008
C4	0.0034	4	0.006
C5	0.0034	4	0.004
C6	0.0034	4	0.002

3. Results and Discussion

To predict the glucose consumption and biohydrogen production, ethanol-type fermentation reactions were included in the species transport and reaction models via the CFD codes. At the beginning of the reaction, mass transfer mainly occurred in the sludge bed region because of liquid–solid mixing (figures 1B and 1C). Then with increasing production and release of biogas, the mass transfer was up-warded.

This was caused by high turbulence due to intensive mixing. Thus, the efficiency of mass transfer is higher than in other regions, meaning that more glucose will be degraded.

Figure 1C presents the mass fraction of hydrogen production, predicted by the CFD simulation of this research. Hydrogen initial production in the bed region to release may be readily seen from this result. The distribution of gas volume fraction is heterogeneous and mainly distributed about the middle. This non-homogeneity is caused by the circular liquid flow under the liquid–gas interaction.

The strategy of operation for the hydrogen production experiments utilizing the laboratory-scale H_2 -producing EGSB reactor was displayed in Table 1. Figures 2A and B show the relationship between the experimental biohydrogen production rate [7] and the outlet hydrogen Mass Flow Rate (MFR) in simulation. From experimental data (see part B of Figure 1) it may be seen that HRT, being related to the water up-flow velocity, affected biohydrogen production. When the HRT exceeded 2h, the hydrodynamic behavior demonstrated was suitable for biohydrogen production. This was due to this behavior which gave an appropriate velocity distribution to maximize inter-phase interactions. By integrating this information with the previous simulation results, a qualitative relationship between hydrodynamics and biohydrogen production might be obtained. In addition, using this reaction model, the response of biohydrogen production with varied inlet mass fraction of glucose in simulation has predictive and directive functions for experimental control and operation (see part A of Figure 1).

4. Conclusions

In this paper, biotreatment of a gas-liquid-solid system has been developed where a CFD code is utilized to investigate its hydrodynamics and reaction kinetics. According to the results of this analysis, the present method is suitable for continuous flow systems. In addition, the results revealed that hydraulic retention time (HRT) have significant effect on hydrogen production. This meant that this factor might be utilized as a key one to control the hydrogen production.

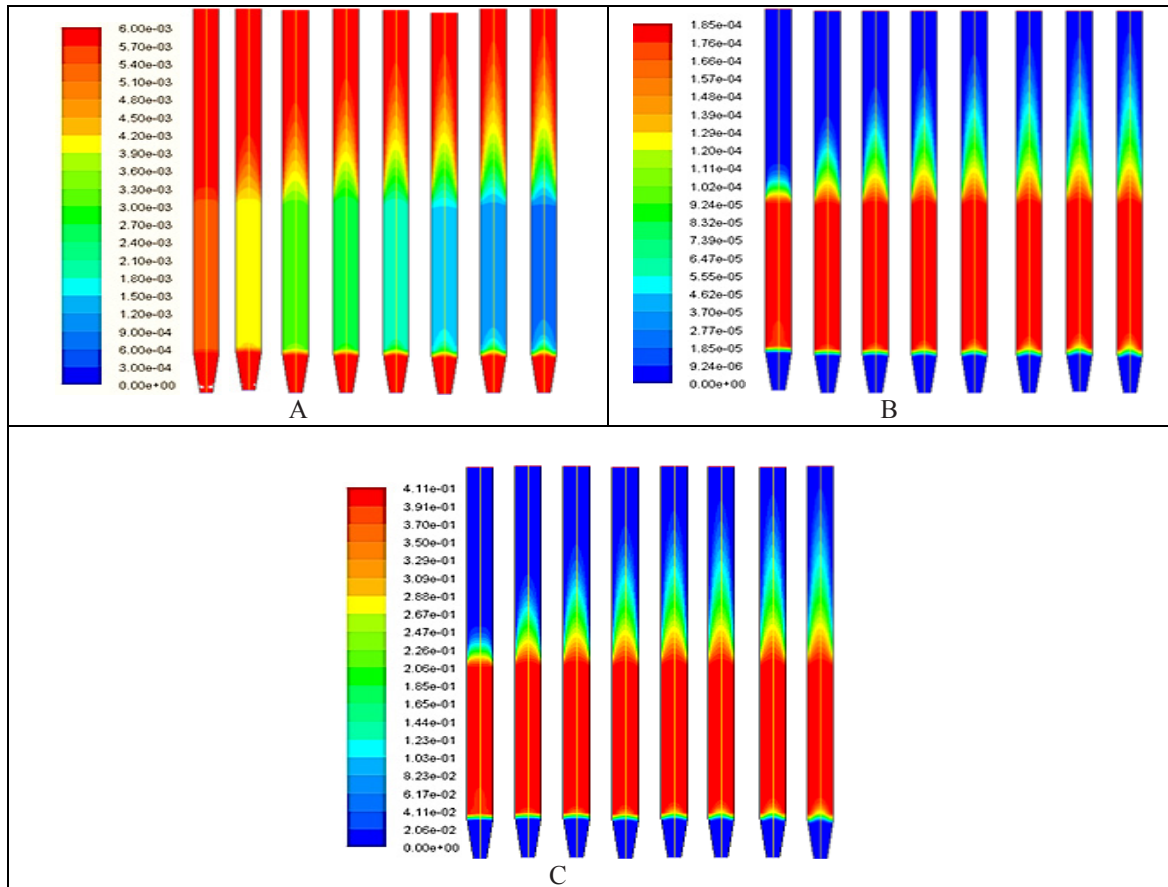


Fig. 1. Contours of species of mass fraction (C4 operating condition) A: Glucose; B: Ethanol; and C: Hydrogen at times of {0.1, 0.3, 0.5, 0.7, 0.9, 1.1, 1.3, 1.5 s}

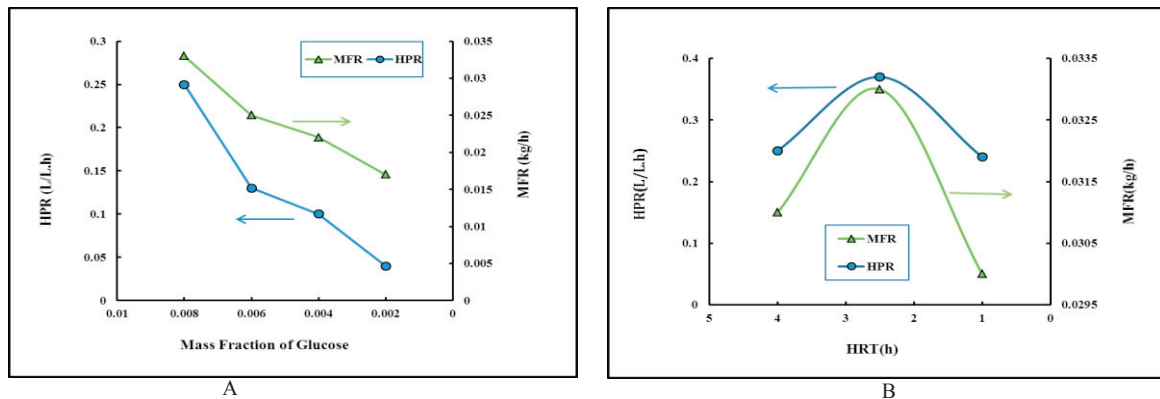


Fig. 2. Experimental and simulated values of the hydrogen production rate with varying MFR, HPR and HRT: A. Constant HRT (4h) and varying mass fraction of glucose; B. Constant mass fraction of glucose (0.008) and varying HRT

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